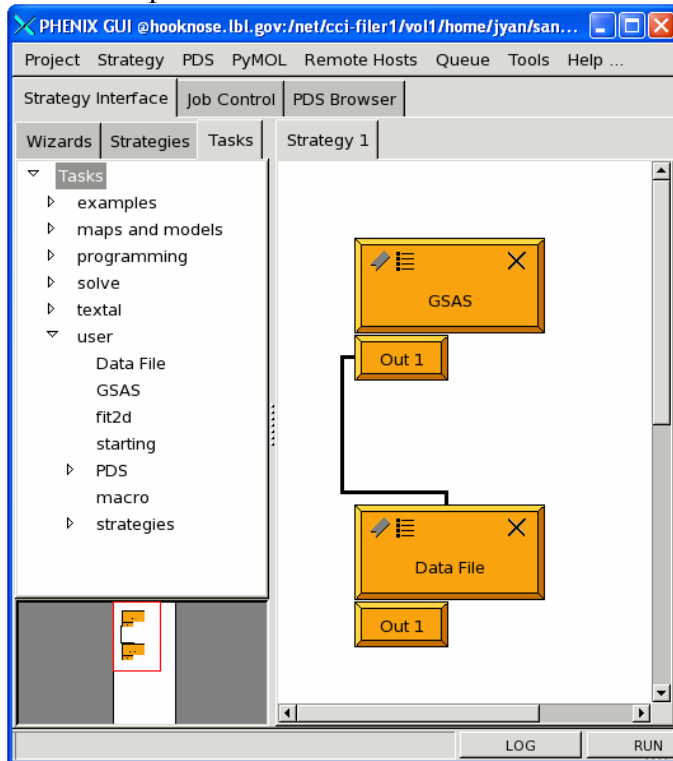


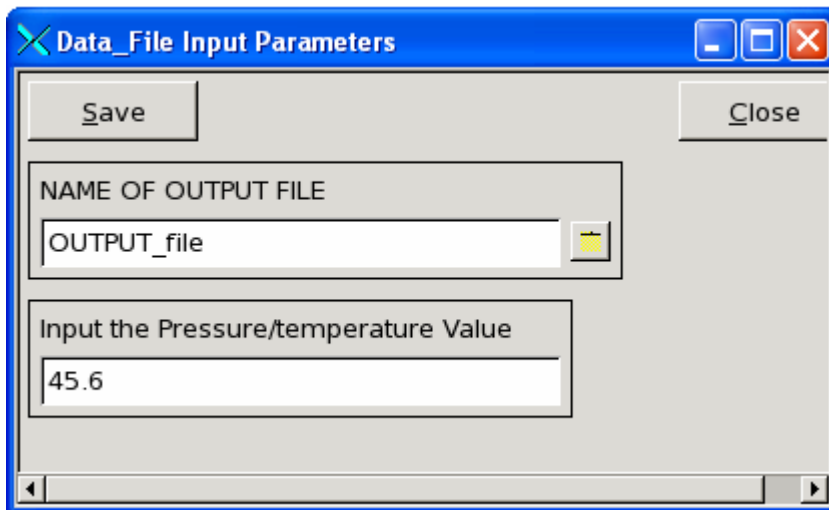
## Monthly Report –July, 2006

My work in the last month focused on automation of GSAS data analysis plus data recording. The raw data (.raw or .gsas) of this example is the one of time of flight of Nickel from the GSAS manual. One PHENIX task code of GSAS data analysis program was developed and a network of both GSAS and data file was created.

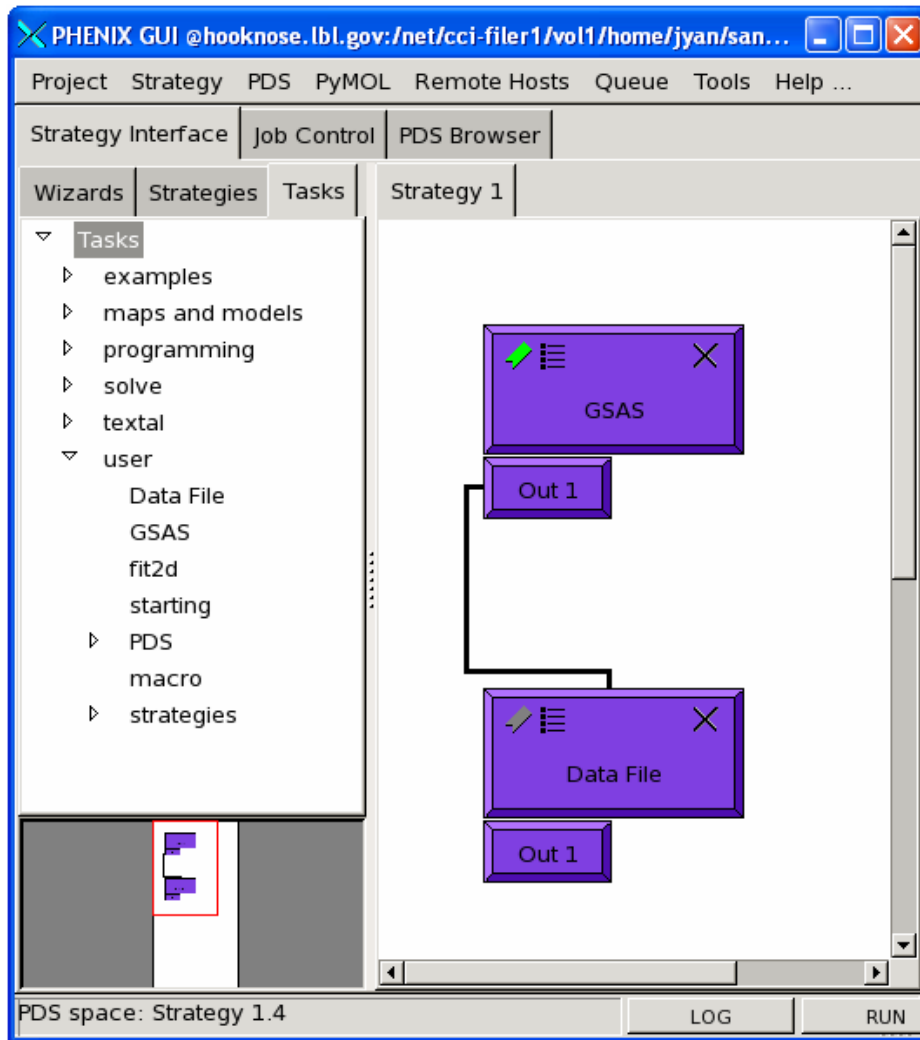


The yellow color in the above window indicates that some required input must finished before running this automation, which are experimental file, raw data from fit2d and instrument in the GSAS task, data record file, and pressure value in the second task.

The screenshot shows the "GSAS Input Parameters" dialog box. It has a "Save" button and a "Close" button. The dialog contains three input fields, each with a file selection icon (a yellow folder with a magnifying glass):  
1. "EXPERIMENTAL FILE" with the text "experimental\_file".  
2. "Raw Data File" with the text "er1/vol1/home/jyan/sandbox/nickel.raw".  
3. "Instrument File" with the text "r1/vol1/home/jyan/sandbox/inst\_tof.prm".

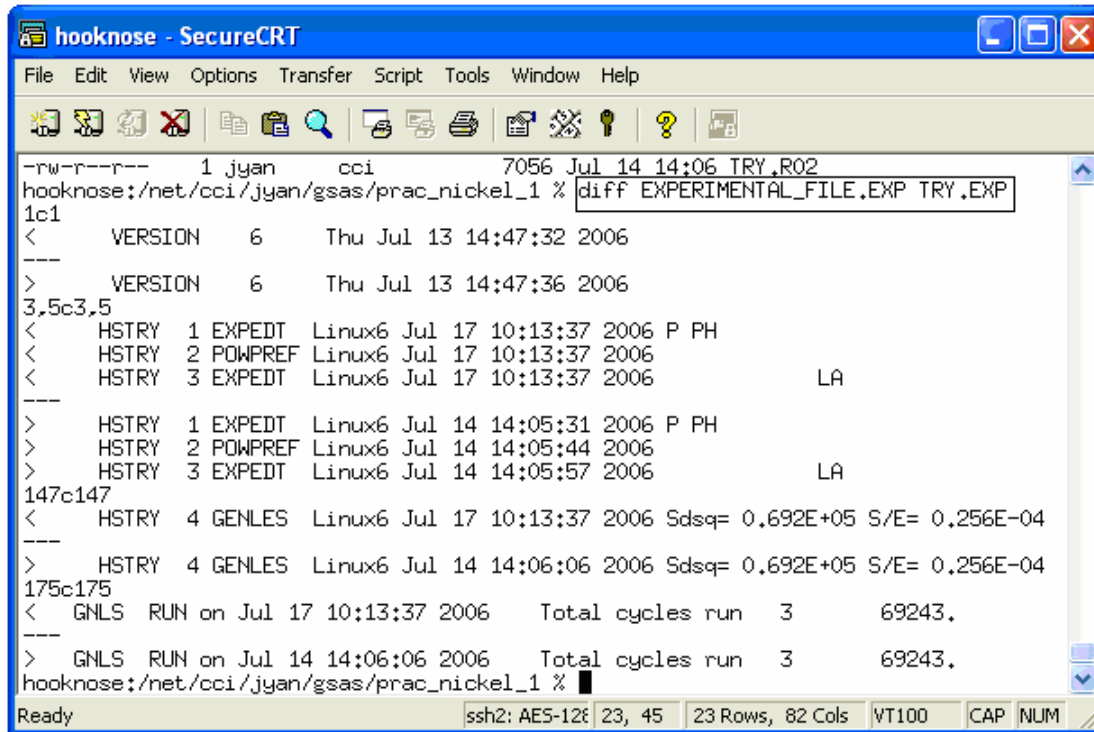


Then, choose the start task (which shows green icon in the below figure), and click the “run” button.



Purple colors tell us the task network has been run successfully.

The experimental file with unit cell information from the above automation is compared with the one from command-line style data analysis using a Linux command “diff”.

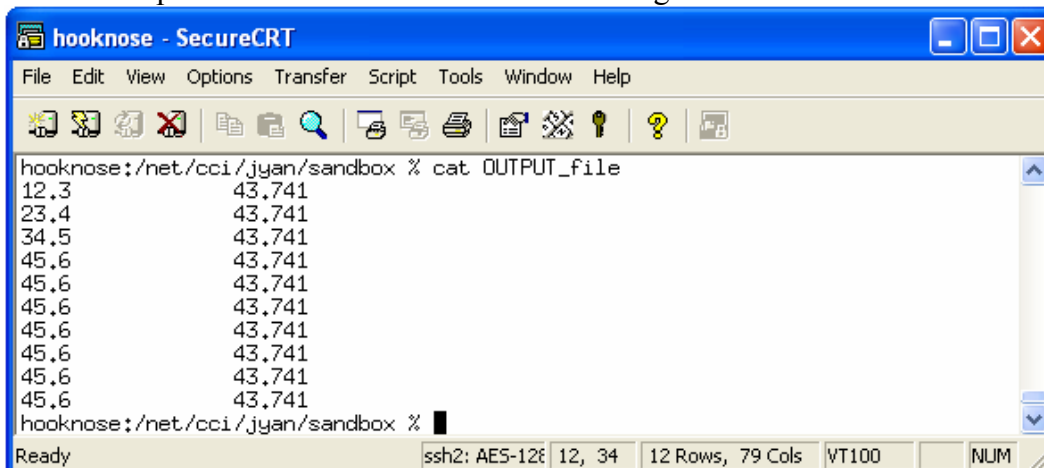


```
hooknose - SecureCRT
File Edit View Options Transfer Script Tools Window Help

-rw-r--r-- 1 jyan cci 7056 Jul 14 14:06 TRY,R02
hooknose:/net/cci/jyan/gsas/prac_nickel_1 % diff EXPERIMENTAL_FILE.EXP TRY.EXP
1c1
< VERSION 6 Thu Jul 13 14:47:32 2006
---
> VERSION 6 Thu Jul 13 14:47:36 2006
3,5c3,5
< HSTRY 1 EXPEDT Linux6 Jul 17 10:13:37 2006 P PH
< HSTRY 2 POWPREF Linux6 Jul 17 10:13:37 2006
< HSTRY 3 EXPEDT Linux6 Jul 17 10:13:37 2006 LA
---
> HSTRY 1 EXPEDT Linux6 Jul 14 14:05:31 2006 P PH
> HSTRY 2 POWPREF Linux6 Jul 14 14:05:44 2006
> HSTRY 3 EXPEDT Linux6 Jul 14 14:05:57 2006 LA
147c147
< HSTRY 4 GENLES Linux6 Jul 17 10:13:37 2006 Sdsq= 0.692E+05 S/E= 0.256E-04
---
> HSTRY 4 GENLES Linux6 Jul 14 14:06:06 2006 Sdsq= 0.692E+05 S/E= 0.256E-04
175c175
< GNLS RUN on Jul 17 10:13:37 2006 Total cycles run 3 69243.
---
> GNLS RUN on Jul 14 14:06:06 2006 Total cycles run 3 69243.
hooknose:/net/cci/jyan/gsas/prac_nickel_1 %
Ready ssh2: AES-128 23, 45 23 Rows, 82 Cols VT100 CAP NUM
```

The above result indicate that the only difference between these two result files are only the running time and date, while all other information of data analysis is exact same.

10 repeatedly running of the automation are preformed with different presumable pressure values but the same raw data file (.gsas file). The recording file with the unit volumes vs pressure values are showed below using a Linux command “cat”.



```
hooknose - SecureCRT
File Edit View Options Transfer Script Tools Window Help

hooknose:/net/cci/jyan/sandbox % cat OUTPUT_file
12.3 43.741
23.4 43.741
34.5 43.741
45.6 43.741
45.6 43.741
45.6 43.741
45.6 43.741
45.6 43.741
45.6 43.741
45.6 43.741
45.6 43.741
hooknose:/net/cci/jyan/sandbox %
Ready ssh2: AES-128 12, 34 12 Rows, 79 Cols VT100 NUM
```

The future work:

1. Try the constant wavelength data example ( LaB6) in addition of TOF.
2. Start work on fit2d program development.
3. Develop the whole CEAD of fit2d, GSAS and plot system.